

Bilayer Rydberg atoms as a quantum simulator for unconventional superconductors.

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We show how systems of cold fermionic Rydberg atoms in a bilayer lattice can be used as a quantum simulator for electron-phonon interactions in the presence of strong electronic correlation: a scenario found in many unconventional superconductors. We discuss the experimental system for making such a simulator, show that the resulting Hamiltonian can be mapped to an extended Hubbard–Holstein model, and make comparison with numerics. Fermions can be simulated, and the proposed quantum simulator can cope with systems where numerics are difficult to apply.

Besides the cuprates, there are several superconductors with high transition temperatures, many of which have important roles for electron-phonon interactions, and repulsion driven correlated electron phenomena such as antiferromagnetism. Fulleride superconductors of the family A_3C_{60} have phonon driven transition temperatures [1] of up to 40K [2], but also exhibit antiferromagnetism at appropriate dopings and structures [3]. Bismuthate superconductors with $T_C > 30K$ [4] have electrons well localized to atomic orbitals with a low density of states at the Fermi surface, with superconductivity probably due to strong couplings to the lattice [5] (as evidenced by a large isotope shift [6, 7]). High transition temperatures have also been achieved in the borocarbides [8, 9] ($T_C = 23K$) and chloronitrides [10] ($T_C = 25K$) which are also thought to be driven by electron-phonon coupling. Even the cuprate superconductors, where superconductivity is thought by many to be driven by antiferromagnetic fluctuations [11], show isotope shifts [12] and other effects such as kinks [13] that may be attributed to some kind of non-trivial interplay between strong correlations and lattice vibrations.

Owing to the importance of electron-phonon interactions in condensed matter, reliable numerical methods have been sought, but even very simplified models [14] are extremely hard to simulate. The difficulty lies in dealing with the potentially infinite number of phonons associated with even a single electron. Another key problem in many advanced materials is that electrons are localized to atomic orbitals and accordingly the Fermi energy is small. This localization means that dimensionless electron-phonon couplings are relatively strong and phonon frequencies can be large at around 10% of the Fermi energy. Even moderate couplings with intermediate frequency phonons can lead to consequences that cannot be predicted with perturbation theory and other analytics. Such couplings can cause additional difficulties for numerics that often work most efficiently in the extreme limits of weak or strong coupling.

Cold atom quantum simulators offer an important new approach to the study of correlated electron phenomena without the limitations of computational or analytical techniques. For example, cold atoms have recently been

used as quantum simulators to investigate standard models of condensed matter physics such as the Hubbard model of strong local Coulomb repulsion [15, 16]. The use of cold atoms to simulate Hubbard models has led to direct observation of important phenomena such as the superfluid to Mott insulator transition [17, 18].

Quantum simulation of lattice effects has proved difficult to implement. The existence of quantum simulators with a high degree of control over the form of interactions has the potential to provide significant insight into the subtle interplay between electronic correlation, lattice vibration and phenomena such as superconductivity and colossal magnetoresistance. In this letter, we propose an approach to simulating fermionic Hubbard models extended to include strong long-range interactions with lattice vibrations, by discussing Rydberg states of cold atoms in bilayer lattices. Such a simulator is likely to shed light on a wide range of unconventional superconductors with transition temperatures greater than 30K, and might resolve some aspects of ongoing debates on cuprate mechanisms. The simulator is introduced and the mapping to a corresponding extended fermionic Hubbard–Holstein model is carried out. We perform simulations to show how the physics of the system is comparable with models of high temperature superconductors. We then discuss how to read properties of the resulting correlated fermion problems from the simulator.

Several schemes for quantum simulation of interactions between electrons and phonons have been suggested. A proposal to bathe an optical lattice in a BEC [19, 20] has led to the observation of polaron effects [21]. Interactions with high energy phonon states of Rydberg ions are used as part of the mapping in proposed simulators for spin systems [22, 23]. Li and Lesanovsky have discussed structural distortions associated with exciting high energy Rydberg states in cold ion crystals [24]. Rydberg atoms have been proposed as a way of simulating polaron effects in strongly deformable materials [25]. The use of cold polar molecules to obtain Holstein polaron effects has been discussed [26]. A scheme for simulation of the Frenkel–Kontorova model to probe friction and energy transport [27] has also been proposed. The scheme

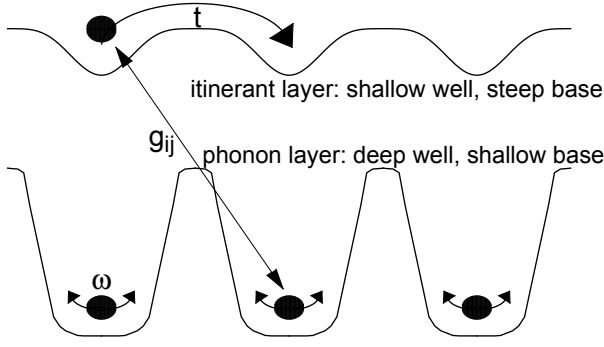


FIG. 1. System of bilayer Rydberg cold atoms for simulation of strong correlations and interactions between fermions and phonons, annotated with Hamiltonian terms.

proposed in this letter goes beyond these as it is capable of simulating interacting Fermions, rather than the interacting Bosons in the earlier schemes.

We begin by discussing how electron-phonon interactions can be simulated in a system of cold, highly excited (Rydberg) atoms in a bilayer lattice. We assume that the Rydberg atoms interact only via dipole-dipole interactions of the form:

$$V_{kl} = -\frac{\mu^2}{|\mathbf{R}_k - \mathbf{R}_l|^3}, \quad (1)$$

where μ is the dipole moment on the Rydberg atom and \mathbf{R}_k is the vector to the k th atom in the lattice. The dipole moment may be written in terms of the coefficient C_3 as $\mu = \sqrt{2}C_3$, and depends upon the Rydberg states chosen for the experiment. The ground state atoms have no long range interaction. By coupling the ground and Rydberg states with a laser tuned Δ from the $|g\rangle \rightarrow |r\rangle$ transition and with coupling strength Ω (the Rabi frequency) we mix the states $|s\rangle$ and $|r\rangle$. This technique [28] of dressing the atoms with the laser means that the trapped, ground state atoms acquire the characteristics of the Rydberg state, but in a controllable fashion. In particular, the coefficient C_3 is replaced by an effective interaction coefficient which we write as $C_3 \rightarrow (\Omega/2\Delta)C_3$.

The atoms, must now be confined in a bilayer lattice. The “itinerant” layer represents e.g. the electrons in a condensed matter problem, and the “phonon” layer acts as a means of simulating the long range interactions between electrons. For the purposes of this model, the itinerant layer may be partially filled, but it is essential that tunneling between adjacent sites is allowed. It is equally important that the phonon layer is completely filled (with 1 atom per site) and that the tunneling is forbidden - the Mott insulator phase [17]. This is achieved by making the potential barrier in the itinerant layer smaller than in the phonon layer. A further complication arises because the atoms in the phonon layer must be set with low oscillating frequencies, while the itinerant layer must be set up

with high phonon frequencies. This can be achieved if the optical lattice in the phonon layer has a special configuration as seen in Fig. 1. This form may be achieved using painted potentials [29] or by superimposing higher order harmonics on a standard optical lattice.

In the itinerant layer, fermions hop with amplitude t , and experience local Coulomb repulsion, U , as in a typical optical lattice experiment to simulate a Hubbard model. Lattice vibrations can be introduced to this system by displacing the atoms in the phonon layer. Atomic displacements do not affect the optical lattice, so the vibrations of the atoms are momentum independent Einstein phonons with Hamiltonian,

$$H_{\text{ph}} = \sum_{\nu} \hbar\omega_{\mathbf{k}\nu} (d_{\nu\mathbf{k}}^\dagger d_{\nu\mathbf{k}} + 1/2). \quad (2)$$

and with polarization vectors $\boldsymbol{\xi}_{\mathbf{k}\nu} = \boldsymbol{\xi}_\nu$ in orthogonal directions. Here $\omega_{\mathbf{k},\nu} = \omega_\nu$ is the angular frequency of a phonon from mode ν with momentum \mathbf{k} and d^\dagger and d respectively represent creation and annihilation operators for phonons. One interesting possibility in 2D is to distort the harmonic potential of the optical lattice to lift the degeneracy of the phonon modes. Also, the use of very distorted potentials allows the probing of anharmonic effects.

The introduction of small in-plane phonon displacements, \mathbf{u}_i , at site i causes the interaction between Rydberg states to become, $V_{kl} = -\Omega^2\mu^2/4\Delta^2|\mathbf{R}_k + \mathbf{u}_k - \mathbf{R}_l - \mathbf{u}_l|^3$, which can be Taylor expanded if the displacement is small,

$$V(\mathbf{R} + \mathbf{u}) \approx \frac{\Omega^2\mu^2}{4\Delta^2|\mathbf{R}|^3} - \frac{3\Omega^2\mu^2\mathbf{u} \cdot \hat{\mathbf{R}}}{4\Delta^2|\mathbf{R}|^4}. \quad (3)$$

The phonon fields can be quantized in the usual way by substituting $\mathbf{u}_i = \sum_{\mathbf{k},\nu} \sqrt{\hbar/2NM\omega_{\mathbf{k},\nu}} \boldsymbol{\xi}_{\mathbf{k},\nu} (d_{\mathbf{k},\nu} e^{-i\mathbf{k} \cdot \mathbf{R}_i} + d_{\mathbf{k},\nu}^\dagger e^{i\mathbf{k} \cdot \mathbf{R}_i})$. Taking into account that all sites in the phonon layer are occupied, and utilizing the momentum independent modes, a multimode extended Hubbard-Holstein interaction is derived,

$$H_{\text{ext-Hol}} = \frac{3\mu^2\Omega^2}{4\Delta^2} \sum_{\nu} \sum_{ij} \hat{\mathbf{R}}_{ij} \cdot \boldsymbol{\xi}_\nu n_i (d_{j,\nu}^\dagger + d_{j,\nu}) / R_{ij}^4 \quad (4)$$

Here, \mathbf{R}_{ij} is a vector between an atom in the itinerant layer at site i , and an atom in the phonon layer at site j , n_i is the number operator for fermions on site i and M is the mass of the atoms. The multimode nature is of particular interest because interaction with multiple phonon modes is difficult to simulate with current numerical techniques.

A further simplification can be made by elongating the potentials in the phonon layer along the direction perpendicular to the planes, so that the Hamiltonian simplifies to the form,

$$H_{\text{Holstein}} = \sum_{ij} g_{ij} n_i (d_j^\dagger + d_j) \quad (5)$$

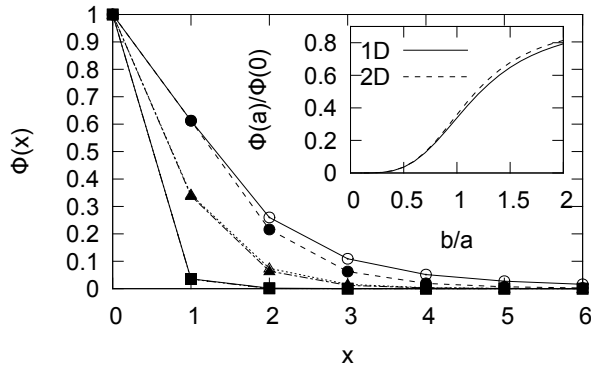


FIG. 2. Comparison between Rydberg and Fröhlich interactions for $\Phi(x)/\Phi(0)$ and various interplane distances. An excellent correspondence between the interactions can be seen for interplane distance $b \lesssim a$. Open points indicate the screened lattice Fröhlich interaction and filled points inter-plane Rydberg interaction. Curves are shown in pairs corresponding to the same $\Phi(a)/\Phi(0)$, so that $R_{sc} \rightarrow \infty$ corresponds to $b = 1.4218(0)a$ (circles), $R_{sc} = 1.4624(5)$ corresponds to $b = a$ (triangles) and $R_{sc} = 0.33233(6)$ to $b = a/2$ (squares).

with the interaction,

$$g_{ij} = \frac{\Omega^2}{4\Delta^2} \frac{3\mu^2 b}{(b^2 + r_{ij}^2)^{5/2}}. \quad (6)$$

where r_{ij} is the distance between the projection of sites i and j onto the same layer and b is the interplane distance. For comparison, a standard Holstein model, where the local electron density couples to local optical phonon modes [14], has $g_{ij} = g\delta_{ij}$. The Fröhlich model describing the continuum limit of interactions between electrons and strongly polarizable materials [30] can be generalized to lattice models and has the form $g_{ij} \sim \exp(-r_{ij}/R_{sc})(b^2 + r_{ij}^2)^{-3/2}$ where R_{sc} is a screening radius[31] (the latter are sometimes known as extended Holstein interactions).

The effective instantaneous interaction between fermions in the itinerant layer is $\Phi(\mathbf{r}) = \sum_{\mathbf{m}} g_{\mathbf{r},\mathbf{m}} g_{0,\mathbf{m}}$. Fig. 2 shows a comparison between the shapes of Rydberg and lattice Fröhlich effective interactions $\Phi(xa)/\Phi(0)$ for various interplane distances and screening radii. As would be done in the experiment, the near-neighbor interactions are matched by modifying b to get the closest possible correspondence to the Fröhlich interaction that is to be simulated. An excellent correspondence between the shapes of the interactions can be seen for interplane distance $b \lesssim a$. The inset shows the near-neighbor interaction for a range of b , for use as a reference to match other types of interaction.

To demonstrate the scheme at relatively low phonon frequencies $\hbar\omega = t$, we use quantum Monte Carlo to compute the properties of polarons and bipolarons in the bilayer lattice and compare with results from the screened

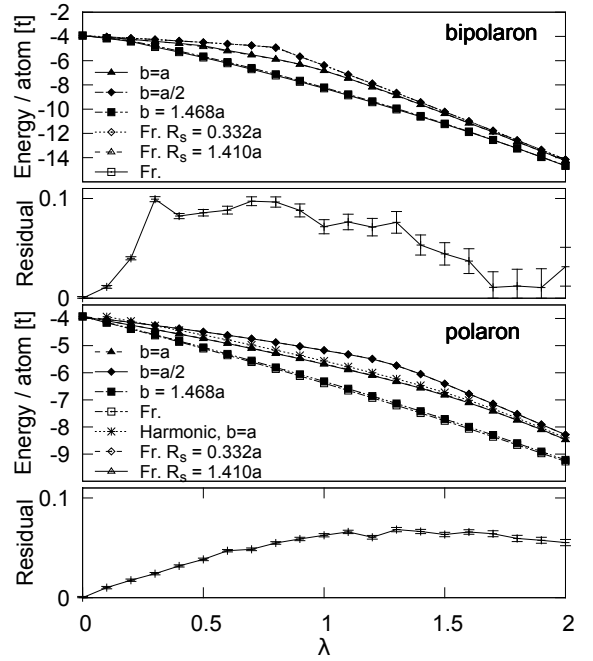


FIG. 3. Polaron and bipolaron energies for different ranges of interaction within the Rydberg scheme proposed here, and for a screened Fröhlich interaction where the near-neighbor interaction strengths have been matched. There is excellent agreement between the two schemes, demonstrating the efficacy of the simulator. Unless shown, error bars are smaller than the points. The lower plots show the residual between the Rydberg and Fröhlich schemes.

Fröhlich interaction. Results from the simulations can be seen in Fig. 3. We also show the effects of the harmonic potentials used in conventional optical lattice schemes. For the low density system simulated, the harmonic potential makes little difference to the overall values of energy and phonon occupation. A very close agreement is found between the quantum simulator and Fröhlich system, further demonstrating the efficacy of our proposal. A key point here is that the quantum simulator is not limited to the low density regime, and will be able to probe and tune key physics of unconventional superconductors at intermediate densities where there is most controversy about the mechanisms.

Finally, we discuss some of the technical challenges which must be solved in order to realize this system. We expect that the simplest implementation would be in an optical lattice setup. So far, micron sized optical traps have been demonstrated, together with direct imaging of single atoms on each lattice site [32]. Recently it has become possible to measure electronic dispersions [33]. Using optical lattices to create the bilayer system presents many challenges, in particular, the need for the two lattices to be as close a few wavelengths of the light λ_l , ideally $1.4\lambda_l$. At the same time, the atoms in one of the lattices must be in the Mott insulating phase, whereas

the other must have appreciable tunneling. In present experimental systems, tunneling between sites occurs when the lattice spacing λ_l is around $0.5 \mu\text{m}$, which is comparable to the diffraction limited spot size of any imaging system used to create the bilayer lattice.

Alternatively, a bilayer optical lattice may be set up with painted potentials [29], a powerful technique with a high level of control over the shapes of features in the optical lattice. Creating a bilayer painted lattice requires two focused horizontal sheets and beams focused between the sheets to form wider features in the phonon layer sheet than the itinerant layer sheet. While the painted potential scheme is harder to implement than traditional optical lattices, it avoids the need to deal with harmonic frequencies.

In the bilayer system, the interesting physics are encoded in the momentum distribution of the gas held in the itinerant layer. What we want to study is the correlation function $C(\mathbf{k}, \sigma; -\mathbf{k}, -\sigma)$. To extract this, the momentum distribution must be observable. In the experiments in Ref. 34, this was accomplished using a time-of-flight method, where the momentum distribution of the roaming atoms is mapped onto the spatial location at the time of imaging.

One further complication arises from employing a dressed atom-atom interaction. In the cases where the two atoms in the itinerant layer occupy a single lattice site, the dipole-dipole interaction may saturate to a constant value, independent of the atomic separation. Following reference [28] we find that the separation R_c at which this occurs is given as $R_c = (C_3/2\hbar|\Delta|)^{1/3}$ (in this expression, C_3 is the undressed C_3 coefficient). This means working with relatively low principal quantum number $n \approx 20$ where the undressed coefficient $C_3 \approx 10 \text{ GHz } \mu\text{m}^3$. In such a case, the atoms will interact as desired for lattices of period greater than 300 nm , but atoms sitting on top of each other will feel a spatially independent interaction. If necessary, the dimensionless interaction strength can be increased by lowering t by making deeper wells in the optical lattice.

In this letter, we have shown how systems of cold Rydberg atoms in a bilayer can be used as a simulator for electron-phonon interactions in the presence of strong electronic correlation, of the type found in many unconventional superconductors. We have carried out the mapping to an extended Hubbard-Holstein model and discussed the experimental requirements for constructing such a simulator. Using continuous-time quantum Monte Carlo simulations, we have shown that results from the simulator are comparable to a Hubbard-Fröhlich model and determined further constraints on the mapping. Furthermore, we have discussed how the simulator can be achieved using contemporary techniques. The proposed quantum simulations system goes well beyond the possibilities of previously proposed quantum simulators for

the simulation of interactions with lattice vibrations. In particular, fermions can be simulated, arbitrary fermion density is achievable, and multiple phonon modes can easily be included.

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- [1] A. Hebard et al. *Nature*, 350:600, 1991.
 - [2] T.T.M. Palstra et al. *Solid St. Commun.*, 93:327, 1995.
 - [3] A.Y. Ganin et al. *Nature*, 466:221, 2010.
 - [4] R.J. Cava et al. *Nature*, 332:814, 1988.
 - [5] I.B. Bischofs, V.N. Kostur, and P.B. Allen. *Phys. Rev. B*, 65:115112, 2002.
 - [6] B. Batlogg et al. *Phys. Rev. Lett.*, 41:1670, 1988.
 - [7] D.G. Hinks et al. *Nature*, 335:419, 1988.
 - [8] R.J. Cava et al. *Nature*, 367:146, 1994.
 - [9] Z. Hossain et al. *Solid State Commun*, 92:341, 1994.
 - [10] H. Kawaji S. Yamanaka, K. Hotehama. *Nature*, 392:580, 1998.
 - [11] P.W. Anderson. *The Theory of Superconductivity in the Cuprates*. Princeton University, Princeton NY, 1997.
 - [12] G.M.Zhao et al. *J. Phys.: Condens. Matter*, 13:R569, 2001.
 - [13] A. Lanzara et al. *Nature*, 412:6846, 2001.
 - [14] T. Holstein. *Ann. Phys.*, 8:325, 1959.
 - [15] J. Hubbard. *Proc. R. Soc. A*, 276:238, 1963.
 - [16] I. Bloch, J. Dalibard, and W. Zwerger. *Rev. Mod. Phys.*, 80:885, 2008.
 - [17] M. Greiner et al. *Nature*, 415:39, 2002.
 - [18] G. K. Campbell et al. *Science*, 313:649, 2006.
 - [19] M. Bruderer, A. Klein, S. R. Clark, and D. Jaksch. *Phys. Rev. A*, 76:011605(R), 2007.
 - [20] M. Bruderer et al. *Phys. Rev. A*, 82:043617, 2010.
 - [21] B. Gadway, D. Pertot, R. Reimann, and D. Schneble. *Phys. Rev. Lett.*, 105:045303, 2010.
 - [22] D. Porras and J. I. Cirac. *Phys. Rev. Lett.*, 92:207901, 2004.
 - [23] M. Müller, L. Liang, I. Lesanovsky, and P. Zoller. *New J. Phys.*, 10:093009, 2008.
 - [24] W. Li and I. Lesanovsky. *arXiv:1108.3591*, 2011.
 - [25] J.P. Hague and C. MacCormick. *arXiv:1109.1225*, 2011.
 - [26] F. Herrera and R. V. Krems. *Phys. Rev. A*, 84:051401, 2011.
 - [27] T. Pruttivarasin et al. *New J. Phys.*, 13:075012, 2011.
 - [28] N. Henkel, R. Nath, and T. Pohl. *Physical Review Letters*, 104:195302, 2010.
 - [29] K. Henderson, C. Ryu, C. MacCormick, and M.G. Boshier. *New Journal of Physics*, 11:043030, 2009.
 - [30] H. Fröhlich. *Proc. Roy. Soc. A*, 215:291, 1952.
 - [31] A.S. Alexandrov and P.E. Kornilovitch. *Phys. Rev. Lett.*, 82:807, 1999.
 - [32] W. S. Bakr et al. *Nature*, 462:74, 2009.
 - [33] J. Heinze et al. *Phys. Rev. Lett.*, 107:135303, 2011.
 - [34] W. S. Bakr et al. *Science*, 329:547, 2010.